FY04 PFC discretionary-funding: LLNL proposals

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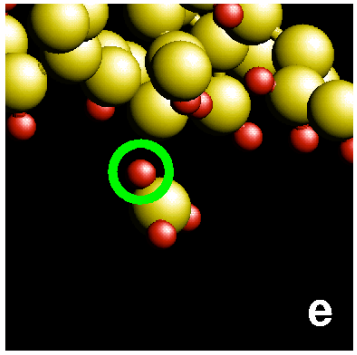

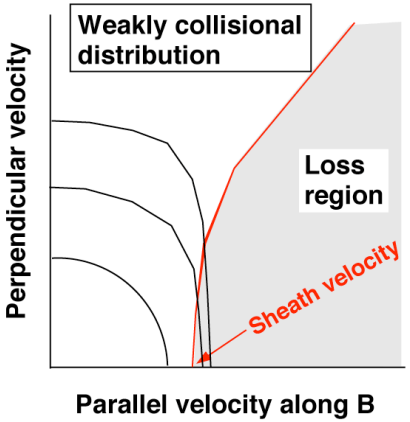

PFC meeting
Oakbrook, November 2003

Proposals for improved MD & SOL plasma modeling

1. **Bringa et al., parallelize AIREBO-potential MD code for hydrocarbon sputtering ($15k)**

2. **Matte et al., kinetic transport for SOL plasmas ($30k)**

Chemical sputtering yields for carbon PFCs have large uncertainties that need to be resolved

- Experimental data yield varied results
- More fundamental understanding is possible through Molecular Dynamics (MD) simulations
- Potential structure is key for MD and important advances have been made
- AIREBO potential includes long-range forces

1. Status & plans for AIREBO at present funding

- Source code already obtained directly from the author (S. Stuart, Clemson University) as part of MD package.
- Add capabilities to do ion bombardment. Code is serial and ~50 times slower than REBO I

- Serial version will be used to generate relaxed samples (graphite+aC:H) as initial conditions for further studies.
- Calculate sputtering yield for one energy and compare to REBO I results (Salonen *et al*, Allain *et al*, etc.). 10 eV D → graphite.

AIREBO utility will be greatly improved by parallelization (add $15k)

- Implement parallel version of AIREBO

- Have arranged collaboration with S. Zybin (Georgetown University)

2. Kinetic SOL plasma transport (add $30k)

Motivation

- **Kinetic transport effects important for steep gradients and/or long mean-free paths**
- **Standard local heat-flux limits are only first approximation**
- **Substantial non-Maxwellian electron tails strongly affect atomic physics rates**
- **Full kinetic codes are available for benchmarking, but very time-consuming**
- **Nonlocal models for parallel electron heat flux, q, have been successful in reproducing full kinetic transport**

$$q(x) = \lambda(x)^{-1} \int W(x,x')\, q_{SH}(x')\, dx'$$

Progress this year for implementation in UEDGE

- Ghang-Geun Kim, postdoc at INRS, has worked with LLNL to implement a nonlocal model in UEDGE
- Test cases show the temperature profile & thus plasma characteristics can be substantially modified
- ITER partially-detached plasma has relevant steep Te gradients & modified ionization rates
- However, Canadian funding ends Dec. '03

$30k could fully fund Kim for FY04 at INRS, thus capitalizing on his initial work

Proposed effort will have two components for FY04

1. Complete high-recycling test cases with UEDGE and benchmark with Fokker-Planck kinetic code

2. Extend nonlocal heat-flux model to nonuniform magnetic field, which is especially important for low recycling

   - NSTX with Li, having a large B-field variation, should produced substantial temperature anisotropy, i.e., $T_{\perp} \neq T_{\parallel}$

   - Past simulations and experiments on laser heated plasmas showed that anisotropy (f_2) is positive in the heat front. This was demonstrated by X-ray line polarization measurements.
     [J.C. Kieffer, J.P. Matte, et al., Phys. Rev. Lett., (1992)]